



ELSEVIER

Chemical Physics 196 (1995) 464–468

Chemical
Physics

Author index to volume 195

- Ando, I., see Kuroki, S. 195 (1995) 107
Ando, S., see Kuroki, S. 195 (1995) 107
Atanasov, M., Intraconfigurational transitions in tetrahedral d^2 ions: on the expediency of the ligand field model for transition metal ions in high-oxidations states 195 (1995) 49
Azriel, V.M., G.D. Billing, L.Yu. Rusin and M.B. Sevryuk, A test of the semiclassical Wigner method for the reaction $F + H_2 \rightarrow H + HF$ 195 (1995) 243
Bak, K.L., see Ruud, K. 195 (1995) 157
Baltzer, P., L. Karlsson, M. Lundqvist, B. Wannberg, D.M.P. Holland and M.A. MacDonald, An experimental study of the valence shell photoelectron spectrum of hydrogen sulphide 195 (1995) 403
Beaufils, S., see Rufflé, B. 195 (1995) 339
Beghin, A., T. Stoecklin and J.C. Rayez, Rate constant calculations for atom–diatom reactions involving an open shell atom and a molecule in a Π electronic state: Application to the $C(^3P) + NO(X^2\Pi)$ reaction 195 (1995) 259
Belford, R.L., see Canfield, J.M. 195 (1995) 59
Berengolts, A., E.I. Dashevskaya, E.E. Nikitin and J. Troe, Dynamic orientation of diatomic fragments formed in the decomposition of statistical triatomic complexes. I. Semiclassical study 195 (1995) 271
Berengolts, A., E.I. Dashevskaya, E.E. Nikitin and J. Troe, Dynamic orientation of diatomic fragments formed in the decomposition of statistical triatomic complexes. II. Classical simulation 195 (1995) 283
Bertault, M., see Longeville, S. 195 (1995) 371
Billing, G.D., see Azriel, V.M. 195 (1995) 243
Borrás-Almenar, J.J., J.M. Clemente, E. Coronado and B.S. Tsukerblat, Mixed-valence polyoxometalate clusters. I. Delocalization of electronic pairs in dodecanuclear heteropoly blues with Keggin structure 195 (1995) 1
Borrás-Almenar, J.J., J.M. Clemente, E. Coronado and B.S. Tsukerblat, Mixed-valence polyoxometalate clusters. II. Delocalization of electronic pairs in 18-site heteropoly blues with Wells–Dawson structure 195 (1995) 17
Borrás-Almenar, J.J., J.M. Clemente, E. Coronado and B.S. Tsukerblat, Mixed-valence polyoxometalate clusters. III. Vibronic problem for the 2-electron reduced heteropoly blue with the Keggin structure 195 (1995) 29
Borsenberger, P.M., W.T. Gruenbaum, E.H. Magin and L.J. Sorriero, Hole transport in tri-*p*-tolylamine doped polymers: the role of the polymer dipole moment 195 (1995) 435
Brec, R., see Sourisseau, C. 195 (1995) 351
Canfield, J.M., R.L. Belford, P.G. Debrunner and K. Schulten, A perturbation treatment of oscillating magnetic fields in the radical pair mechanism using the Liouville equation 195 (1995) 59

- Cavagnat, R., see Sourisseau, C. 195 (1995) 351
- Chajia, M. and M. Jacon, The effect of rotational excitation on the reaction $^{18}\text{O}(^3\text{P}) + ^{16}\text{O}^{16}\text{O}(^3\Sigma_g^-) \rightarrow ^{18}\text{O}^{16}\text{O}(^3\Sigma_g^-) + ^{16}\text{O}(^3\text{P})$. A comparison of quasiclassical and hemiquantal hyperspherical dynamics 195 (1995) 195
- Chandra, A., Dielectric relaxation of binary dipolar liquids 195 (1995) 93
- Chang, A., see Dolg, M. 195 (1995) 71
- Chronister, E.L., see L'Espérance, D. 195 (1995) 387
- Clemente, J.M., see Borrás-Almenar, J.J. 195 (1995) 1
- Clemente, J.M., see Borrás-Almenar, J.J. 195 (1995) 17
- Clemente, J.M., see Borrás-Almenar, J.J. 195 (1995) 29
- Coronado, E., see Borrás-Almenar, J.J. 195 (1995) 1
- Coronado, E., see Borrás-Almenar, J.J. 195 (1995) 17
- Coronado, E., see Borrás-Almenar, J.J. 195 (1995) 29
- Dashevskaya, E.I., see Berengolts, A. 195 (1995) 271
- Dashevskaya, E.I., see Berengolts, A. 195 (1995) 283
- Davister, M., see Loch, R. 195 (1995) 443
- De Alti, G., see Fronzoni, G. 195 (1995) 171
- Debrunner, P.G., see Canfield, J.M. 195 (1995) 59
- Decleva, P., see Fronzoni, G. 195 (1995) 171
- Delugeard, Y., see Longeville, S. 195 (1995) 371
- Dolg, M., P. Fulde, H. Stoll, H. Preuss, A. Chang and R.M. Pitzer, Formally tetravalent cerium and thorium compounds: a configuration interaction study of cerocene $\text{Ce}(\text{C}_8\text{H}_8)_2$ and thorocene $\text{Th}(\text{C}_8\text{H}_8)_2$ using energy-adjusted quasirelativistic ab initio pseudopotentials 195 (1995) 71
- Eichler, H.J., R. Macdonald, R. Menzel and R. Sander, Excited state absorption of 5CB (4'-n-pentyl-4-cyanobiphenyl) in cyclohexane 195 (1995) 381
- Elder, S.H., see Sourisseau, C. 195 (1995) 351
- Esteban, M., see Garay, M. 195 (1995) 235
- Even, J., see Longeville, S. 195 (1995) 371
- Fave, J.L., see Longeville, S. 195 (1995) 371
- Felder, P., see Gejo, T. 195 (1995) 423
- Floris, F., M. Persico, A. Tani and J. Tomasi, Free energies and structures of hydrated cations, based on effective pair potentials 195 (1995) 207
- Fouassier, M., see Sourisseau, C. 195 (1995) 351
- Fronzoni, G., G. De Alti, P. Decleva and A. Lisini, Correlation effects in core and valence photoelectron spectra of alkene molecules 195 (1995) 171
- Fulde, P., see Dolg, M. 195 (1995) 71
- Gallier, J., see Rufflé, B. 195 (1995) 339
- Garay, M., M. Esteban, E. Verdasco and A. González Ureña, Reaction cross-section and product polarization in the $\text{Ca}(^1\text{D}_2) + \text{HBr} \rightarrow \text{CaBr}(\text{A,B}) + \text{H}$ reaction 195 (1995) 235
- Gejo, T., P. Felder and J.R. Huber, The concerted photodissociation of azomethane at 193 nm 195 (1995) 423
- Girard, A., see Longeville, S. 195 (1995) 371

- Gonzales, D.A. and P.L. Varghese, Vibrational relaxation models for dilute shock heated gases 195 (1995) 83
- González Ureña, A., see Garay, M. 195 (1995) 235
- Gruenbaum, W.T., see Borsenberger, P.M. 195 (1995) 435
- Hawks, M.R., R.O. Johnson and G.P. Perram, Infrared fluorescence study of electronic-to-vibrational energy transfer in the $\text{Br}(^2\text{P}_{1/2})\text{-NO}$ system 195 (1995) 395
- Hawlicka, E. and D. Swiatla-Wojcik, Molecular dynamics studies on the structure of methanol-water solutions of NaCl 195 (1995) 221
- Helgaker, T., see Ruud, K. 195 (1995) 157
- Henry, B.R., see Turnbull, D.M. 195 (1995) 129
- Holland, D.M.P., see Baltzer, P. 195 (1995) 403
- Huber, J.R., see Gejo, T. 195 (1995) 423
- Jacon, M., see Chajia, M. 195 (1995) 195
- Johnson, R.O., see Hawks, M.R. 195 (1995) 395
- Jørgensen, P., see Ruud, K. 195 (1995) 157
- Karlsson, L., see Baltzer, P. 195 (1995) 403
- Katoh, R., K. Lacmann and W.F. Schmidt, Effect of high pressure on photoionization of N,N,N',N'-tetramethyl-*p*-phenylenediamine (TMPD) in liquid 2,2-dimethylbutane (DMB) 195 (1995) 457
- Kjaergaard, H.G., see Turnbull, D.M. 195 (1995) 129
- Korolev, V.V., see Vasenkov, S.V. 195 (1995) 305
- Kuroki, S., S. Ando and I. Ando, An MO study of nuclear quadrupolar coupling constant and nuclear shielding of the carbonyl oxygen in solid peptides with hydrogen bonds 195 (1995) 107
- Lacmann, K., see Katoh, R. 195 (1995) 457
- L'Espérance, D. and E.L. Chronister, Dispersive electronic energy transfer in an organically doped xerogel glass 195 (1995) 387
- Lisini, A., see Fronzoni, G. 195 (1995) 171
- Locht, R. and M. Davister, The dissociative ionization of C_2H_2 . The C^+ , C_2^+ and CH_2^+ dissociation channels. The vinylidene ion as a transient? 195 (1995) 443
- Longeville, S., M. Bertault, J. Even, J.L. Fave, A. Girard and Y. Delugeard, A Raman study of the disorder induced by polymer chains in mixed monomer-polymer crystals of the diacetylene pTS-D 195 (1995) 371
- Ludwig, R., NMR relaxation studies in water-alcohol mixtures: the water-rich region 195 (1995) 329
- Lundqvist, M., see Baltzer, P. 195 (1995) 403
- MacDonald, M.A., see Baltzer, P. 195 (1995) 403
- Macdonald, R., see Eichler, H.J. 195 (1995) 381
- Magin, E.H., see Borsenberger, P.M. 195 (1995) 435
- Menzel, R., see Eichler, H.J. 195 (1995) 381
- Nikitin, E.E., see Berengolts, A. 195 (1995) 271
- Nikitin, E.E., see Berengolts, A. 195 (1995) 283
- Olsen, J., see Ruud, K. 195 (1995) 157

- Perram, G.P., see Hawks, M.R. 195 (1995) 395
- Persico, M., see Floris, F. 195 (1995) 207
- Persky, A., see Rosenman, E. 195 (1995) 291
- Pitzer, R.M., see Dolg, M. 195 (1995) 71
- Preuss, H., see Dolg, M. 195 (1995) 71
- Rayez, J.C., see Beghin, A. 195 (1995) 259
- Rosenman, E. and A. Persky, Quasiclassical trajectory study of the $F + H_2$ system. Rate constants, kinetic isotope effects and energy partitioning among reaction products 195 (1995) 291
- Rufflé, B., S. Beaufils and J. Gallier, Low-frequency motions in an alkali phosphate glass studied by 7Li and ^{31}P NMR 195 (1995) 339
- Rusin, L.Yu., see Azriel, V.M. 195 (1995) 243
- Ruud, K., T. Helgaker, K.L. Bak, P. Jørgensen and J. Olsen, Accurate magnetizabilities of the isoelectronic series BeH^- , BH , and CH^+ . The MCSCF-GIAO approach 195 (1995) 157
- Sander, R., see Eichler, H.J. 195 (1995) 381
- Schmidt, W.F., see Katoh, R. 195 (1995) 457
- Schulten, K., see Canfield, J.M. 195 (1995) 59
- Sevryuk, M.B., see Azriel, V.M. 195 (1995) 243
- Sorriero, L.J., see Borsenberger, P.M. 195 (1995) 435
- Sourisseau, C., R. Cavagnat, M. Fouassier, R. Brec and S.H. Elder, Infrared, Raman, resonance Raman spectra and lattice dynamics calculations of the solid potassium(I) nickel(II) thiophosphate compound, $KNiPS_4$ 195 (1995) 351
- Springborg, M., On solitonic defects in hydrogen-bonded $(HF)_x$ 195 (1995) 143
- Stoecklin, T., see Beghin, A. 195 (1995) 259
- Stoll, H., see Dolg, M. 195 (1995) 71
- Swiatla-Wojcik, D., see Hawlicka, E. 195 (1995) 221
- Takeshita, K., A theoretical study on the ionic states, with analysis of vibrational levels of the photoelectron spectrum, of formic acid (CH_2O_2 and CD_2O_2) 195 (1995) 117
- Tani, A., see Floris, F. 195 (1995) 207
- Tolkatchev, V.A., see Vasenkov, S.V. 195 (1995) 305
- Tolkatchev, V.A., see Vyazovkin, V.L. 195 (1995) 313
- Tomasi, J., see Floris, F. 195 (1995) 207
- Troe, J., see Berengolts, A. 195 (1995) 271
- Troe, J., see Berengolts, A. 195 (1995) 283
- Tsukerblat, B.S., see Borrás-Almenar, J.J. 195 (1995) 1
- Tsukerblat, B.S., see Borrás-Almenar, J.J. 195 (1995) 17
- Tsukerblat, B.S., see Borrás-Almenar, J.J. 195 (1995) 29
- Turnbull, D.M., H.G. Kjaergaard and B.R. Henry, Intensities of CH-stretching overtones in 2-butenes 195 (1995) 129
- Varghese, P.L., see Gonzales, D.A. 195 (1995) 83
- Vasenkov, S.V., V.V. Korolev and V.A. Tolkatchev, The influence of deep traps for gas molecules on oxygen transport in the glass of 2-methylpentanol-2 195 (1995) 305
- Verdasco, E., see Garay, M. 195 (1995) 235
- Vyazovkin, V.L. and V.A. Tolkatchev, H-atom abstraction from alcohols by alkyl radicals. Cooperative effects in the reactions of alkyl radicals in glassy methanol- d_3 195 (1995) 313
- Wannberg, B., see Baltzer, P. 195 (1995) 403



Subject index to volume 195

Methods

Theoretical

Group theory and algebras

- Mixed-valence polyoxometalate clusters. I. Delocalization of electronic pairs in dodecanuclear heteropoly blues with Keggin structure, J.J. Borrás-Almenar, J.M. Clemente, E. Coronado and B.S. Tsukerblat 195 (1995) 1
- Mixed-valence polyoxometalate clusters. II. Delocalization of electronic pairs in 18-site heteropoly blues with Wells–Dawson structure, J.J. Borrás-Almenar, J.M. Clemente, E. Coronado and B.S. Tsukerblat 195 (1995) 17

Many body and quasiparticle approaches

- Intraconfigurational transitions in tetrahedral d^2 ions: on the expediency of the ligand field model for transition metal ions in high-oxidations states, M. Atanasov 195 (1995) 49

Coupling schemes and perturbative treatments

- Mixed-valence polyoxometalate clusters. III. Vibronic problem for the 2-electron reduced heteropoly blue with the Keggin structure, J.J. Borrás-Almenar, J.M. Clemente, E. Coronado and B.S. Tsukerblat 195 (1995) 29
- A perturbation treatment of oscillating magnetic fields in the radical pair mechanism using the Liouville equation, J.M. Canfield, R.L. Belford, P.G. Debrunner and K. Schulten 195 (1995) 59

Relativistic quantum mechanics

- Formally tetravalent cerium and thorium compounds: a configuration interaction study of cerocene $Ce(C_8H_8)_2$ and thorocene $Th(C_8H_8)_2$ using energy-adjusted quasirelativistic ab initio pseudopotentials, M. Dolg, P. Fulde, H. Stoll, H. Preuss, A. Chang and R.M. Pitzer 195 (1995) 71

Non-equilibrium thermodynamic and hydrodynamic theories

- Vibrational relaxation models for dilute shock heated gases, D.A. Gonzales and P.L. Varghese 195 (1995) 83
- Dielectric relaxation of binary dipolar liquids, A. Chandra 195 (1995) 93

Ab initio schemes for stationary properties

- An MO study of nuclear quadrupolar coupling constant and nuclear shielding of the carbonyl oxygen in solid peptides with hydrogen bonds, S. Kuroki, S. Ando and I. Ando 195 (1995) 107
- A theoretical study on the ionic states, with analysis of vibrational levels of the photoelectron spectrum, of formic acid (CH_2O_2 and CD_2O_2), K. Takeshita 195 (1995) 117
- Intensities of CH-stretching overtones in 2-butenes, D.M. Turnbull, H.G. Kjaergaard and B.R. Henry 195 (1995) 129
- On solitonic defects in hydrogen-bonded $(\text{HF})_x$, M. Springborg 195 (1995) 143
- Accurate magnetizabilities of the isoelectronic series BeH^- , BH , and CH^+ . The MCSCF-GIAO approach, K. Ruud, T. Helgaker, K.L. Bak, P. Jørgensen and J. Olsen 195 (1995) 157
- Correlation effects in core and valence photoelectron spectra of alkene molecules, G. Fronzoni, G. De Alti, P. Decleva and A. Lisini 195 (1995) 171

Computational and simulation methods

- Vibrational relaxation models for dilute shock heated gases, D.A. Gonzales and P.L. Varghese 195 (1995) 83
- The effect of rotational excitation on the reaction $^{18}\text{O}(^3\text{P}) + ^{16}\text{O}^{16}\text{O}(^3\Sigma_g^-) \rightarrow ^{18}\text{O}^{16}\text{O}(^3\Sigma_g^-) + ^{16}\text{O}(^3\text{P})$. A comparison of quasiclassical and hemiquantal hyperspherical dynamics, M. Chajia and M. Jacon 195 (1995) 195
- Free energies and structures of hydrated cations, based on effective pair potentials, F. Floris, M. Persico, A. Tani and J. Tomasi 195 (1995) 207
- Molecular dynamics studies on the structure of methanol–water solutions of NaCl, E. Hawlicka and D. Swiatla-Wojcik 195 (1995) 221

Molecular dynamics and scattering theory

- The effect of rotational excitation on the reaction $^{18}\text{O}(^3\text{P}) + ^{16}\text{O}^{16}\text{O}(^3\Sigma_g^-) \rightarrow ^{18}\text{O}^{16}\text{O}(^3\Sigma_g^-) + ^{16}\text{O}(^3\text{P})$. A comparison of quasiclassical and hemiquantal hyperspherical dynamics, M. Chajia and M. Jacon 195 (1995) 195
- Reaction cross-section and product polarization in the $\text{Ca}(^1\text{D}_2) + \text{HBr} \rightarrow \text{CaBr}(\text{A,B}) + \text{H}$ reaction, M. Garay, M. Esteban, E. Verdasco and A. González Ureña 195 (1995) 235
- A test of the semiclassical Wigner method for the reaction $\text{F} + \text{H}_2 \rightarrow \text{H} + \text{HF}$, V.M. Azriel, G.D. Billing, L.Yu. Rusin and M.B. Sevryuk 195 (1995) 243
- Rate constant calculations for atom–diatom reactions involving an open shell atom and a molecule in a Π electronic state: Application to the $\text{C}(^3\text{P}) + \text{NO}(^2\Pi)$ reaction, A. Beghin, T. Stoecklin and J.C. Rayez 195 (1995) 259
- Dynamic orientation of diatomic fragments formed in the decomposition of statistical triatomic complexes. I. Semiclassical study, A. Berengolts, E.I. Dashevskaya, E.E. Nikitin and J. Troe 195 (1995) 271
- Dynamic orientation of diatomic fragments formed in the decomposition of statistical triatomic complexes. II. Classical simulation, A. Berengolts, E.I. Dashevskaya, E.E. Nikitin and J. Troe 195 (1995) 283
- Quasiclassical trajectory study of the $\text{F} + \text{H}_2$ system. Rate constants, kinetic isotope effects and energy partitioning among reaction products, E. Rosenman and A. Persky 195 (1995) 291

Experimental*Magnetic resonances*

- An MO study of nuclear quadrupolar coupling constant and nuclear shielding of the carbonyl oxygen in solid peptides with hydrogen bonds, S. Kuroki, S. Ando and I. Ando 195 (1995) 107

- The influence of deep traps for gas molecules on oxygen transport in the glass of 2-methylpentanol-2, S.V. Vasenkov, V.V. Korolev and V.A. Tolkatchev 195 (1995) 305
- H-atom abstraction from alcohols by alkyl radicals. Cooperative effects in the reactions of alkyl radicals in glassy methanol- d_3 , V.L. Vyazovkin and V.A. Tolkatchev 195 (1995) 313
- NMR relaxation studies in water-alcohol mixtures: the water-rich region, R. Ludwig 195 (1995) 329
- Low-frequency motions in an alkali phosphate glass studied by ^7Li and ^{31}P NMR, B. Rufflé, S. Beaufils and J. Gallier 195 (1995) 339

Infrared spectroscopy

- Infrared, Raman, resonance Raman spectra and lattice dynamics calculations of the solid potassium(I) nickel(II) thiophosphate compound, KNiPS_4 , C. Sourisseau, R. Cavagnat, M. Fouassier, R. Brec and S.H. Elder 195 (1995) 351

Raman spectroscopy

- Infrared, Raman, resonance Raman spectra and lattice dynamics calculations of the solid potassium(I) nickel(II) thiophosphate compound, KNiPS_4 , C. Sourisseau, R. Cavagnat, M. Fouassier, R. Brec and S.H. Elder 195 (1995) 351
- A Raman study of the disorder induced by polymer chains in mixed monomer-polymer crystals of the diacetylene pTS-D, S. Longeville, M. Bertault, J. Even, J.L. Fave, A. Girard and Y. Delugeard 195 (1995) 371

Visible and UV spectroscopy

- Excited state absorption of 5CB (4'-n-pentyl-4-cyanobiphenyl) in cyclohexane, H.J. Eichler, R. Macdonald, R. Menzel and R. Sander 195 (1995) 381

Fluorescence spectroscopy

- Reaction cross-section and product polarization in the $\text{Ca}(^1\text{D}_2) + \text{HBr} \rightarrow \text{CaBr}(\text{A,B}) + \text{H}$ reaction, M. Garay, M. Esteban, E. Verdasco and A. González Ureña 195 (1995) 235
- The influence of deep traps for gas molecules on oxygen transport in the glass of 2-methylpentanol-2, S.V. Vasenkov, V.V. Korolev and V.A. Tolkatchev 195 (1995) 305
- Dispersive electronic energy transfer in an organically doped xerogel glass, D. L'Espérance and E.L. Chronister 195 (1995) 387
- Infrared fluorescence study of electronic-to-vibrational energy transfer in the $\text{Br}(^2\text{P}_{1/2})\text{-NO}$ system, M.R. Hawks, R.O. Johnson and G.P. Perram 195 (1995) 395

Photoelectron and Auger spectroscopy

- A theoretical study on the ionic states, with analysis of vibrational levels of the photoelectron spectrum, of formic acid (CH_2O_2 and CD_2O_2), K. Takeshita 195 (1995) 117
- An experimental study of the valence shell photoelectron spectrum of hydrogen sulphide, P. Baltzer, L. Karlsson, M. Lundqvist, B. Wannberg, D.M.P. Holland and M.A. Macdonald 195 (1995) 403

Laser methods

- Intensities of CH-stretching overtones in 2-butenes, D.M. Turnbull, H.G. Kjaergaard and B.R. Henry 195 (1995) 129
- The concerted photodissociation of azomethane at 193 nm, T. Gejo, P. Felder and J.R. Huber 195 (1995) 423

Non-linear optical spectroscopy

- Excited state absorption of 5CB (4'-*n*-pentyl-4-cyanobiphenyl) in cyclohexane, H.J. Eichler, R. Macdonald, R. Menzel and R. Sander 195 (1995) 381

Synchrotron spectroscopies

- An experimental study of the valence shell photoelectron spectrum of hydrogen sulphide, P. Baltzer, L. Karlsson, M. Lundqvist, B. Wannberg, D.M.P. Holland and M.A. MacDonald 195 (1995) 403

Atomic and molecular beam techniques

- The concerted photodissociation of azomethane at 193 nm, T. Gejo, P. Felder and J.R. Huber 195 (1995) 423

Time-resolved experiments

- Dispersive electronic energy transfer in an organically doped xerogel glass, D. L'Espérance and E.L. Chronister 195 (1995) 387
- Hole transport in tri-*p*-tolylamine doped polymers: the role of the polymer dipole moment, P.M. Borsenberger, W.T. Gruenbaum, E.H. Magin and L.J. Sorriero 195 (1995) 435

Mass spectrometry

- The dissociative ionization of C_2H_2 . The C^+ , C_2^+ and CH_2^+ dissociation channels. The vinylidene ion as a transient?, R. Locht and M. Davister 195 (1995) 443

Radiolysis

- H-atom abstraction from alcohols by alkyl radicals. Cooperative effects in the reactions of alkyl radicals in glassy methanol- d_3 , V.L. Vyazovkin and V.A. Tolkmachev 195 (1995) 313

Measurement of macroscopic variables

- Effect of high pressure on photoionization of N,N,N',N'-tetramethyl-*p*-phenylenediamine (TMPD) in liquid 2,2-dimethylbutane (DMB), R. Katoh, K. Lacmann and W.F. Schmidt 195 (1995) 457

Objects**Bulk systems***Gases*

- Vibrational relaxation models for dilute shock heated gases, D.A. Gonzales and P.L. Varghese 195 (1995) 83
- A test of the semiclassical Wigner method for the reaction $F + H_2 \rightarrow H + HF$, V.M. Azriel, G.D. Billing, L.Yu. Rusin and M.B. Sevryuk 195 (1995) 243
- The dissociative ionization of C_2H_2 . The C^+ , C_2^+ and CH_2^+ dissociation channels. The vinylidene ion as a transient?, R. Locht and M. Davister 195 (1995) 443

Supersonic beams

- The concerted photodissociation of azomethane at 193 nm, T. Gejo, P. Felder and J.R. Huber 195 (1995) 423

Liquid mixtures and solutions

- Dielectric relaxation of binary dipolar liquids, A. Chandra 195 (1995) 93
- Free energies and structures of hydrated cations, based on effective pair potentials, F. Floris, M. Persico, A. Tani and J. Tomasi 195 (1995) 207
- Molecular dynamics studies on the structure of methanol–water solutions of NaCl, E. Hawlicka and D. Swiatla-Wojcik 195 (1995) 221
- NMR relaxation studies in water–alcohol mixtures: the water-rich region, R. Ludwig 195 (1995) 329
- Effect of high pressure on photoionization of N,N,N',N'-tetramethyl-*p*-phenylenediamine (TMPD) in liquid 2,2-dimethylbutane (DMB), R. Katoh, K. Lacmann and W.F. Schmidt 195 (1995) 457

*Crystals**-mixed*

- A Raman study of the disorder induced by polymer chains in mixed monomer–polymer crystals of the diacetylene pTS-D, S. Longeville, M. Bertault, J. Even, J.L. Fave, A. Girard and Y. Delugeard 195 (1995) 371

Glasses

- The influence of deep traps for gas molecules on oxygen transport in the glass of 2-methylpentanol-2, S.V. Vasenkov, V.V. Korolev and V.A. Tolkatchev 195 (1995) 305
- H-atom abstraction from alcohols by alkyl radicals. Cooperative effects in the reactions of alkyl radicals in glassy methanol-*d*₃, V.L. Vyazovkin and V.A. Tolkatchev 195 (1995) 313
- Low-frequency motions in an alkali phosphate glass studied by ⁷Li and ³¹P NMR, B. Rufflé, S. Beaufils and J. Gallier 195 (1995) 339
- Dispersive electronic energy transfer in an organically doped xerogel glass, D. L'Espérance and E.L. Chronister 195 (1995) 387

Liquid crystals

- Excited state absorption of 5CB (4'-*n*-pentyl-4-cyanobiphenyl) in cyclohexane, H.J. Eichler, R. Macdonald, R. Menzel and R. Sander 195 (1995) 381

Polymers

- An MO study of nuclear quadrupolar coupling constant and nuclear shielding of the carbonyl oxygen in solid peptides with hydrogen bonds, S. Kuroki, S. Ando and I. Ando 195 (1995) 107
- A Raman study of the disorder induced by polymer chains in mixed monomer–polymer crystals of the diacetylene pTS-D, S. Longeville, M. Bertault, J. Even, J.L. Fave, A. Girard and Y. Delugeard 195 (1995) 371
- Hole transport in tri-*p*-tolylamine doped polymers: the role of the polymer dipole moment, P.M. Borsenberger, W.T. Gruenbaum, E.H. Magin and L.J. Sorriero 195 (1995) 435

Low-dimensional materials

- On solitonic defects in hydrogen-bonded (HF)_x, M. Springborg 195 (1995) 143
- Infrared, Raman, resonance Raman spectra and lattice dynamics calculations of the solid potassium(I) nickel(II) thiophosphate compound, KNiPS₄, C. Sourisseau, R. Cavagnat, M. Fouassier, R. Brec and S.H. Elder 195 (1995) 351

Biological systems

- A perturbation treatment of oscillating magnetic fields in the radical pair mechanism using the Liouville equation, J.M. Canfield, R.L. Belford, P.G. Debrunner and K. Schulten 195 (1995) 59

Microscopic systems*Atoms*

- Infrared fluorescence study of electronic-to-vibrational energy transfer in the $\text{Br}(^2\text{P}_{1/2})\text{-NO}$ system, M.R. Hawks, R.O. Johnson and G.P. Perram 195 (1995) 395

Molecules (neutral and ionic)

- Formally tetravalent cerium and thorium compounds: a configuration interaction study of cerocene $\text{Ce}(\text{C}_8\text{H}_8)_2$ and thorocene $\text{Th}(\text{C}_8\text{H}_8)_2$ using energy-adjusted quasirelativistic ab initio pseudopotentials, M. Dolg, P. Fulde, H. Stoll, H. Preuss, A. Chang and R.M. Pitzer 195 (1995) 71
- Accurate magnetizabilities of the isoelectronic series BeH^- , BH , and CH^+ . The MCSCF-GIAO approach, K. Ruud, T. Helgaker, K.L. Bak, P. Jørgensen and J. Olsen 195 (1995) 157
- Correlation effects in core and valence photoelectron spectra of alkene molecules, G. Fronzoni, G. De Alti, P. Decleva and A. Lisini 195 (1995) 171
- The effect of rotational excitation on the reaction $^{18}\text{O}(^3\text{P}) + ^{16}\text{O}^{16}\text{O}(^3\Sigma_g^-) \rightarrow ^{18}\text{O}^{16}\text{O}(^3\Sigma_g^-) + ^{16}\text{O}(^3\text{P})$. A comparison of quasiclassical and hemiquantal hyperspherical dynamics, M. Chajia and M. Jacon 195 (1995) 195
- Reaction cross-section and product polarization in the $\text{Ca}(^1\text{D}_2) + \text{HBr} \rightarrow \text{CaBr}(\text{A,B}) + \text{H}$ reaction, M. Garay, M. Esteban, E. Verdasco and A. González Ureña 195 (1995) 235
- Excited state absorption of 5CB (4'-n-pentyl-4-cyanobiphenyl) in cyclohexane, H.J. Eichler, R. Macdonald, R. Menzel and R. Sander 195 (1995) 381

-diatomic

- Accurate magnetizabilities of the isoelectronic series BeH^- , BH , and CH^+ . The MCSCF-GIAO approach, K. Ruud, T. Helgaker, K.L. Bak, P. Jørgensen and J. Olsen 195 (1995) 157
- A test of the semiclassical Wigner method for the reaction $\text{F} + \text{H}_2 \rightarrow \text{H} + \text{HF}$, V.M. Azriel, G.D. Billing, L.Yu. Rusin and M.B. Sevryuk 195 (1995) 243
- Rate constant calculations for atom-diatom reactions involving an open shell atom and a molecule in a Π electronic state: Application to the $\text{C}(^3\text{P}) + \text{NO}(^2\Pi)$ reaction, A. Beghin, T. Stoecklin and J.C. Rayez 195 (1995) 259
- Infrared fluorescence study of electronic-to-vibrational energy transfer in the $\text{Br}(^2\text{P}_{1/2})\text{-NO}$ system, M.R. Hawks, R.O. Johnson and G.P. Perram 195 (1995) 395

-small polyatomics

- A theoretical study on the ionic states, with analysis of vibrational levels of the photoelectron spectrum, of formic acid (CH_2O_2 and CD_2O_2), K. Takeshita 195 (1995) 117
- Correlation effects in core and valence photoelectron spectra of alkene molecules, G. Fronzoni, G. De Alti, P. Decleva and A. Lisini 195 (1995) 171
- Dynamic orientation of diatomic fragments formed in the decomposition of statistical triatomic complexes. I. Semiclassical study, A. Berengolts, E.I. Dashevskaya, E.E. Nikitin and J. Troe 195 (1995) 271
- Dynamic orientation of diatomic fragments formed in the decomposition of statistical triatomic complexes. II. Classical simulation, A. Berengolts, E.I. Dashevskaya, E.E. Nikitin and J. Troe 195 (1995) 283
- An experimental study of the valence shell photoelectron spectrum of hydrogen sulphide, P. Baltzer, L. Karlsson, M. Lundqvist, B. Wannberg, D.M.P. Holland and M.A. MacDonal 195 (1995) 403

- The concerted photodissociation of azomethane at 193 nm, T. Gejo, P. Felder and J.R. Huber 195 (1995) 423
- Hole transport in tri-*p*-tolylamine doped polymers: the role of the polymer dipole moment, P.M. Borsenberger, W.T. Gruenbaum, E.H. Magin and L.J. Sorriero 195 (1995) 435
- The dissociative ionization of C_2H_2 . The C^+ , C_2^+ and CH_2^+ dissociation channels. The vinylidene ion as a transient?, R. Locht and M. Davister 195 (1995) 443
- other large*
- Formally tetravalent cerium and thorium compounds: a configuration interaction study of cerocene $Ce(C_8H_8)_2$ and thorocene $Th(C_8H_8)_2$ using energy-adjusted quasirelativistic ab initio pseudopotentials, M. Dolg, P. Fulde, H. Stoll, H. Preuss, A. Chang and R.M. Pitzer 195 (1995) 71
- Intensities of CH-stretching overtones in 2-butenes, D.M. Turnbull, H.G. Kjaergaard and B.R. Henry 195 (1995) 129
- polymeric and biological*
- An MO study of nuclear quadrupolar coupling constant and nuclear shielding of the carbonyl oxygen in solid peptides with hydrogen bonds, S. Kuroki, S. Ando and I. Ando 195 (1995) 107
- Molecular aggregates*
- dimers*
- Dispersive electronic energy transfer in an organically doped xerogel glass, D. L'Espérance and E.L. Chronister 195 (1995) 387
- clusters*
- Mixed-valence polyoxometalate clusters. I. Delocalization of electronic pairs in dodecanuclear heteropoly blues with Keggin structure, J.J. Borrás-Almenar, J.M. Clemente, E. Coronado and B.S. Tsukerblat 195 (1995) 1
- Mixed-valence polyoxometalate clusters. II. Delocalization of electronic pairs in 18-site heteropoly blues with Wells–Dawson structure, J.J. Borrás-Almenar, J.M. Clemente, E. Coronado and B.S. Tsukerblat 195 (1995) 17
- Intraconfigurational transitions in tetrahedral d^2 ions: on the expediency of the ligand field model for transition metal ions in high-oxidations states, M. Atanasov 195 (1995) 49
- complexes*
- Mixed-valence polyoxometalate clusters. I. Delocalization of electronic pairs in dodecanuclear heteropoly blues with Keggin structure, J.J. Borrás-Almenar, J.M. Clemente, E. Coronado and B.S. Tsukerblat 195 (1995) 1
- Mixed-valence polyoxometalate clusters. II. Delocalization of electronic pairs in 18-site heteropoly blues with Wells–Dawson structure, J.J. Borrás-Almenar, J.M. Clemente, E. Coronado and B.S. Tsukerblat 195 (1995) 17
- Intraconfigurational transitions in tetrahedral d^2 ions: on the expediency of the ligand field model for transition metal ions in high-oxidations states, M. Atanasov 195 (1995) 49
- Free radicals (including hydronium and muonium)*
- A perturbation treatment of oscillating magnetic fields in the radical pair mechanism using the Liouville equation, J.M. Canfield, R.L. Belford, P.G. Debrunner and K. Schulten 195 (1995) 59

- Rate constant calculations for atom–diatom reactions involving an open shell atom and a molecule in a Π electronic state: Application to the $C(^3P) + NO(X^2\Pi)$ reaction, A. Beghin, T. Stoecklin and J.C. Rayez 195 (1995) 259
- H-atom abstraction from alcohols by alkyl radicals. Cooperative effects in the reactions of alkyl radicals in glassy methanol- d_3 , V.L. Vyazovkin and V.A. Tolkatchev 195 (1995) 313

Ions and charge carriers

- Free energies and structures of hydrated cations, based on effective pair potentials, F. Floris, M. Persico, A. Tani and J. Tomasi 195 (1995) 207
- Low-frequency motions in an alkali phosphate glass studied by 7Li and ^{31}P NMR, B. Rufflé, S. Beaufils and J. Gallier 195 (1995) 339
- Effect of high pressure on photoionization of N,N,N',N'-tetramethyl-*p*-phenylenediamine (TMPD) in liquid 2,2-dimethylbutane (DMB), R. Katoh, K. Lacmann and W.F. Schmidt 195 (1995) 457

Phenomena

Molecular structure

- Formally tetravalent cerium and thorium compounds: a configuration interaction study of cerocene $Ce(C_8H_8)_2$ and thorocene $Th(C_8H_8)_2$ using energy-adjusted quasirelativistic ab initio pseudopotentials, M. Dolg, P. Fulde, H. Stoll, H. Preuss, A. Chang and R.M. Pitzer 195 (1995) 71
- Accurate magnetizabilities of the isoelectronic series BeH^- , BH , and CH^+ . The MCSCF-GIAO approach, K. Ruud, T. Helgaker, K.L. Bak, P. Jørgensen and J. Olsen 195 (1995) 157
- NMR relaxation studies in water-alcohol mixtures: the water-rich region, R. Ludwig 195 (1995) 329

Vibrations and rotations of molecules

- A theoretical study on the ionic states, with analysis of vibrational levels of the photoelectron spectrum, of formic acid (CH_2O_2 and CD_2O_2), K. Takeshita 195 (1995) 117
- Intensities of CH-stretching overtones in 2-butenes, D.M. Turnbull, H.G. Kjaergaard and B.R. Henry 195 (1995) 129

Electronic structure and states

- Intraconfigurational transitions in tetrahedral d^2 ions: on the expediency of the ligand field model for transition metal ions in high-oxidations states, M. Atanasov 195 (1995) 49
- Formally tetravalent cerium and thorium compounds: a configuration interaction study of cerocene $Ce(C_8H_8)_2$ and thorocene $Th(C_8H_8)_2$ using energy-adjusted quasirelativistic ab initio pseudopotentials, M. Dolg, P. Fulde, H. Stoll, H. Preuss, A. Chang and R.M. Pitzer 195 (1995) 71
- On solitonic defects in hydrogen-bonded $(HF)_x$, M. Springborg 195 (1995) 143
- Infrared, Raman, resonance Raman spectra and lattice dynamics calculations of the solid potassium(I) nickel(II) thiophosphate compound, $KNiPS_4$, C. Sourisseau, R. Cavagnat, M. Fouassier, R. Brec and S.H. Elder 195 (1995) 351
- Excited state absorption of 5CB (4'-*n*-pentyl-4-cyanobiphenyl) in cyclohexane, H.J. Eichler, R. Macdonald, R. Menzel and R. Sander 195 (1995) 381
- An experimental study of the valence shell photoelectron spectrum of hydrogen sulphide, P. Baltzer, L. Karlsson, M. Lundqvist, B. Wannberg, D.M.P. Holland and M.A. Mac-Donald 195 (1995) 403

Electric and magnetic properties

- Mixed-valence polyoxometalate clusters. I. Delocalization of electronic pairs in dodecanuclear heteropoly blues with Keggin structure, J.J. Borrás-Almenar, J.M. Clemente, E. Coronado and B.S. Tsukerblat 195 (1995) 1
- Mixed-valence polyoxometalate clusters. II. Delocalization of electronic pairs in 18-site heteropoly blues with Wells–Dawson structure, J.J. Borrás-Almenar, J.M. Clemente, E. Coronado and B.S. Tsukerblat 195 (1995) 17
- Mixed-valence polyoxometalate clusters. III. Vibronic problem for the 2-electron reduced heteropoly blue with the Keggin structure, J.J. Borrás-Almenar, J.M. Clemente, E. Coronado and B.S. Tsukerblat 195 (1995) 29
- A perturbation treatment of oscillating magnetic fields in the radical pair mechanism using the Liouville equation, J.M. Canfield, R.L. Belford, P.G. Debrunner and K. Schulten 195 (1995) 59
- An MO study of nuclear quadrupolar coupling constant and nuclear shielding of the carbonyl oxygen in solid peptides with hydrogen bonds, S. Kuroki, S. Ando and I. Ando 195 (1995) 107
- Accurate magnetizabilities of the isoelectronic series BeH^- , BH , and CH^+ . The MCSCF-GIAO approach, K. Ruud, T. Helgaker, K.L. Bak, P. Jørgensen and J. Olsen 195 (1995) 157
- Hole transport in tri-*p*-tolylamine doped polymers: the role of the polymer dipole moment, P.M. Borsenberger, W.T. Gruenbaum, E.H. Magin and L.J. Sorriero 195 (1995) 435

Molecular interactions

- Quasiclassical trajectory study of the $\text{F} + \text{H}_2$ system. Rate constants, kinetic isotope effects and energy partitioning among reaction products, E. Rosenman and A. Persky 195 (1995) 291

Spectral bandshapes and intensities

- A perturbation treatment of oscillating magnetic fields in the radical pair mechanism using the Liouville equation, J.M. Canfield, R.L. Belford, P.G. Debrunner and K. Schulten 195 (1995) 59
- Intensities of CH-stretching overtones in 2-butenes, D.M. Turnbull, H.G. Kjaergaard and B.R. Henry 195 (1995) 129

Coupling of electronic and nuclear motion

- Mixed-valence polyoxometalate clusters. III. Vibronic problem for the 2-electron reduced heteropoly blue with the Keggin structure, J.J. Borrás-Almenar, J.M. Clemente, E. Coronado and B.S. Tsukerblat 195 (1995) 29

Energy transfer processes

- Dispersive electronic energy transfer in an organically doped xerogel glass, D. L'Espérance and E.L. Chronister 195 (1995) 387
- Infrared fluorescence study of electronic-to-vibrational energy transfer in the $\text{Br}(^2\text{P}_{1/2})\text{--NO}$ system, M.R. Hawks, R.O. Johnson and G.P. Perram 195 (1995) 395

Molecular photophysical processes

- Infrared fluorescence study of electronic-to-vibrational energy transfer in the $\text{Br}(^2\text{P}_{1/2})\text{--NO}$ system, M.R. Hawks, R.O. Johnson and G.P. Perram 195 (1995) 395
- An experimental study of the valence shell photoelectron spectrum of hydrogen sulphide, P. Baltzer, L. Karlsson, M. Lundqvist, B. Wannberg, D.M.P. Holland and M.A. MacDonald 195 (1995) 403
- Effect of high pressure on photoionization of N,N,N',N' -tetramethyl-*p*-phenylenediamine (TMPD) in liquid 2,2-dimethylbutane (DMB), R. Katoh, K. Lacmann and W.F. Schmidt 195 (1995) 457

Intramolecular dynamics

- Infrared, Raman, resonance Raman spectra and lattice dynamics calculations of the solid potassium(I) nickel(II) thiophosphate compound, KNiPS_4 , C. Sourisseau, R. Cavagnat, M. Fouassier, R. Brec and S.H. Elder 195 (1995) 351

Luminescence spectra, yields and lifetimes

- Intraconfigurational transitions in tetrahedral d^2 ions: on the expediency of the ligand field model for transition metal ions in high-oxidations states, M. Atanasov 195 (1995) 49
- Reaction cross-section and product polarization in the $\text{Ca}(^1D_2) + \text{HBr} \rightarrow \text{CaBr(A,B)} + \text{H}$ reaction, M. Garay, M. Esteban, E. Verdasco and A. González Ureña 195 (1995) 235

Reactions (including dissociation)

- Vibrational relaxation models for dilute shock heated gases, D.A. Gonzales and P.L. Varghese 195 (1995) 83
- Reaction cross-section and product polarization in the $\text{Ca}(^1D_2) + \text{HBr} \rightarrow \text{CaBr(A,B)} + \text{H}$ reaction, M. Garay, M. Esteban, E. Verdasco and A. González Ureña 195 (1995) 235
- Rate constant calculations for atom-diatom reactions involving an open shell atom and a molecule in a Π electronic state: Application to the $\text{C}(^3P) + \text{NO}(X^2\Pi)$ reaction, A. Beghin, T. Stoecklin and J.C. Rayez 195 (1995) 259

-gas phase

- Vibrational relaxation models for dilute shock heated gases, D.A. Gonzales and P.L. Varghese 195 (1995) 83
- The effect of rotational excitation on the reaction $^{18}\text{O}(^3P) + ^{16}\text{O}^{16}\text{O}(^3\Sigma_g^-) \rightarrow ^{18}\text{O}^{16}\text{O}(^3\Sigma_g^-) + ^{16}\text{O}(^3P)$. A comparison of quasiclassical and hemiquantal hyperspherical dynamics, M. Chajia and M. Jacon 195 (1995) 195
- A test of the semiclassical Wigner method for the reaction $\text{F} + \text{H}_2 \rightarrow \text{H} + \text{HF}$, V.M. Azriel, G.D. Billing, L.Yu. Rusin and M.B. Sevryuk 195 (1995) 243
- Rate constant calculations for atom-diatom reactions involving an open shell atom and a molecule in a Π electronic state: Application to the $\text{C}(^3P) + \text{NO}(X^2\Pi)$ reaction, A. Beghin, T. Stoecklin and J.C. Rayez 195 (1995) 259
- Dynamic orientation of diatomic fragments formed in the decomposition of statistical triatomic complexes. I. Semiclassical study, A. Berengolts, E.I. Dashevskaya, E.E. Nikitin and J. Troe 195 (1995) 271
- Dynamic orientation of diatomic fragments formed in the decomposition of statistical triatomic complexes. II. Classical simulation, A. Berengolts, E.I. Dashevskaya, E.E. Nikitin and J. Troe 195 (1995) 283
- Quasiclassical trajectory study of the $\text{F} + \text{H}_2$ system. Rate constants, kinetic isotope effects and energy partitioning among reaction products, E. Rosenman and A. Persky 195 (1995) 291
- The dissociative ionization of C_2H_2 . The C^+ , C_2^+ and CH_2^+ dissociation channels. The vinylidene ion as a transient?, R. Locht and M. Davister 195 (1995) 443

-condensed phase

- The influence of deep traps for gas molecules on oxygen transport in the glass of 2-methylpentanol-2, S.V. Vasenkov, V.V. Korolev and V.A. Tolkatchev 195 (1995) 305

-photochemical

- The concerted photodissociation of azomethane at 193 nm, T. Gejo, P. Felder and J.R. Huber 195 (1995) 423

Tunnelling

- Mixed-valence polyoxometalate clusters. III. Vibronic problem for the 2-electron reduced heteropoly blue with the Keggin structure, J.J. Borrás-Almenar, J.M. Clemente, E. Coronado and B.S. Tsukerblat 195 (1995) 29

Electron transfer

- Mixed-valence polyoxometalate clusters. I. Delocalization of electronic pairs in dodecanuclear heteropoly blues with Keggin structure, J.J. Borrás-Almenar, J.M. Clemente, E. Coronado and B.S. Tsukerblat 195 (1995) 1
- Mixed-valence polyoxometalate clusters. II. Delocalization of electronic pairs in 18-site heteropoly blues with Wells–Dawson structure, J.J. Borrás-Almenar, J.M. Clemente, E. Coronado and B.S. Tsukerblat 195 (1995) 17
- Mixed-valence polyoxometalate clusters. III. Vibronic problem for the 2-electron reduced heteropoly blue with the Keggin structure, J.J. Borrás-Almenar, J.M. Clemente, E. Coronado and B.S. Tsukerblat 195 (1995) 29
- Hole transport in tri-*p*-tolylamine doped polymers: the role of the polymer dipole moment, P.M. Borsenberger, W.T. Gruenbaum, E.H. Magin and L.J. Sorriero 195 (1995) 435

Ionization (including Rydberg states)

- A theoretical study on the ionic states, with analysis of vibrational levels of the photoelectron spectrum, of formic acid (CH_2O_2 and CD_2O_2), K. Takeshita 195 (1995) 117
- Correlation effects in core and valence photoelectron spectra of alkene molecules, G. Fronzoni, G. De Alti, P. Decleva and A. Lisini 195 (1995) 171
- The dissociative ionization of C_2H_2 . The C^+ , C_2^+ and CH_2^+ dissociation channels. The vinylidene ion as a transient?, R. Locht and M. Davister 195 (1995) 443

Molecular motion (including diffusive)

- The influence of deep traps for gas molecules on oxygen transport in the glass of 2-methylpentanol-2, S.V. Vasenkov, V.V. Korolev and V.A. Tolkatchev 195 (1995) 305
- H-atom abstraction from alcohols by alkyl radicals. Cooperative effects in the reactions of alkyl radicals in glassy methanol- d_3 , V.L. Vyazovkin and V.A. Tolkatchev 195 (1995) 313
- NMR relaxation studies in water-alcohol mixtures: the water-rich region, R. Ludwig 195 (1995) 329
- Low-frequency motions in an alkali phosphate glass studied by ^7Li and ^{31}P NMR, B. Rufflé, S. Beaufils and J. Gallier 195 (1995) 339

Isotopic effects

- Quasiclassical trajectory study of the $\text{F} + \text{H}_2$ system. Rate constants, kinetic isotope effects and energy partitioning among reaction products, E. Rosenman and A. Persky 195 (1995) 291

Collective motion and excitations

- Dielectric relaxation of binary dipolar liquids, A. Chandra 195 (1995) 93

Thermodynamic and transport properties

- Free energies and structures of hydrated cations, based on effective pair potentials, F. Floris, M. Persico, A. Tani and J. Tomasi 195 (1995) 207

Phase transitions

- Low-frequency motions in an alkali phosphate glass studied by ^7Li and ^{31}P NMR, B. Rufflé, S. Beaufils and J. Gallier 195 (1995) 339
- A Raman study of the disorder induced by polymer chains in mixed monomer-polymer crystals of the diacetylene pTS-D, S. Longeville, M. Bertault, J. Even, J.L. Fave, A. Girard and Y. Delugeard 195 (1995) 371

